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Impact of advection process in simulating the dynamics of diffusion-controlled irreversible fast/moderate/slow bimolecular-reactive systems

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ABSTRACT

Diffusion-controlled bimolecular reactions arise in various branches of natural sciences [1], chemically reacting systems [2], and contaminant transport [3]. Based on the kinetics of the chemical reaction, they are broadly classified in to three categories: fast, moderate, and slow [4]. Herein, we are interested in the dynamics of a (fast/moderate/slow) bimolecular reaction given by the following stoichiometric relationship [5]:

$$nA A + nB\, B \longrightarrow nC\, C$$

In this discussion, we shall present a computational framework to simulate the dynamics of an irreversible bimolecular advection–diffusion–reaction (ADR) system within the context of low-order mixed finite element method. Most importantly, we shall study the effect of advection process on the formation of product C and its role in understanding fast/moderate/slow chemical reaction kinetics. In continuous setting, it is well-known in the literature on partial differential equations [6–8] that the solution to the governing equations ADR system possesses various important physical and mathematical properties such as non-negativity, maximum principles, comparison principles, monotonicity, and monotone property. Herein, we shall discuss whether such properties are inherited or lost during the procedure of finite element discretization. Furthermore, through various representative examples, we shall quantify the errors incurred in satisfying the local and global species balance property. Finally, we shall provide a general methodology to satisfy all these discrete properties (including local and global species balance property) simultaneously within the context of low-order finite elements.

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